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Irreducible Representations of Groups of Order 8

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Abstract Irreducible representations of a group provide the ways for labelling orbitals, determining molecular orbitals formation and determining vibrational motions for a molecule. A set of irreducible representations represents the ways a particular bond, atom or sets of atoms may respond to a given set of symmetry operations. In this paper, the irreducible representations of all groups of order 8, namely D_4, Q, C_8, $C_2 \times C_4$ and $C_2 \times C_2 \times C_2$ are obtained using Burnside method and Great Orthogonality Theorem method. Then, comparisons of the two methods are made.

Keywords Irreducible representation, group, Burnside method, Great Orthogonality Theorem method.

1 Introduction

There are different ways that individual atoms, bonds, atomic orbitals and any other piece of the overall molecule respond to symmetry operations. Obtaining the irreducible representations associated with a given bond, atoms or sets of atoms is a way of labelling orbitals for reference. Besides, irreducible representations determine which sets of atomic orbitals can combine with each other to form molecular orbitals. Furthermore, an irreducible representation of a molecule determines the number and nature of vibrational motions for the molecule by removing the irreducible representations that correspond to the translation and rotation of the molecule.

There are five groups of order 8 which consist of two non-Abelian groups and three Abelian groups. The groups are all written in group presentation form, that is the form of a group with a set of generators and certain relations for the generators to satisfy.

The first non-Abelian group of order 8 is the dihedral group,

$$D_4 = \langle a, b | a^4 = b^2 = 1, a^b = a^{-1} \rangle.$$

The second non-Abelian group of order 8 is the quaternion group,

$$Q = \langle a, b | a^4 = 1, b^2 = a^2, a^b = a^{-1} \rangle.$$

The first Abelian group of order 8 is the cyclic group, $C_8 = \langle a | a^8 = 1 \rangle$. The second Abelian group of order 8 is the direct product of the groups C_2 with C_4, namely

$$C_2 \times C_4 = \langle a, b | a^2 = b^4 = 1, ab = ba \rangle.$$

The third Abelian group of order 8 is

$$C_2 \times C_2 \times C_2 = \langle a, b, c | a^2 = b^2 = c^2 = 1, ab = ba, ac = ca, bc = cb \rangle.$$

The irreducible representations of all of these groups will be obtained using Burnside method and Great Orthogonality Theorem method. Then, comparisons of the two methods are made.

2 Burnside Method

Burnside method, proposed by Burnside in 1911, can be used to obtain the irreducible representations of a group [1]. Using this method, three formulas are involved in finding the irreducible representations of a group, that is, the irreducible representations k. Using these formulas, class multiplication coefficients, characters of the irreducible representations in terms of d_k and the numerical values for d_k are obtained.

The first step in getting the irreducible representations is to obtain the class multiplication coefficients. Following Cracknell [2], the result of multiplying together two classes C_i and C_j is a sum of several classes C_s:

$$C_i C_j = \sum_s c_{ij,s} C_s \tag{1}$$

where $c_{ij,s}$ are the class multiplication coefficients. Using equation (1), the class multiplication coefficients $c_{ij,s}$ can be evaluated.

The next step is to obtain the characters of the irreducible representations in terms of d_k, where d_k is the dimension of the kth irreducible representation. Following Burns [1], the characters are given in the form of:

$$h_i h_j {\chi_i}^k {\chi_j}^k = d_k \sum_{s=1}^{r} c_{ij,s} h_s {\chi_s}^k \tag{2}$$

where h_i is the order of the class C_i, ${\chi_i}^k$ is the character of the elements in class C_i in the irreducible representation labelled by k, d_k is the dimension of the kth irreducible representation, $c_{ij,s}$ is the class multiplication coefficient and r is the number of classes in the group.

The last step of getting the irreducible representations is to obtain the numerical values for d_k using [2]:

$$\sum_{i=1}^{r} h_i {\chi_i}^j {\chi_i}^k = N \delta_{jk} \tag{3}$$

where N is the order of the group, δ_{jk} is the Kronecker Delta symbol, which has the value 1 when $i = j$, but has the value 0 when $i \neq j$, r is the number of classes in the group, ${\chi_i}^j$ and ${\chi_i}^k$ are the characters of elements in class C_i in the irreducible representation labelled by j and k respectively. The number of irreducible representations of a group is equal to the number of classes [2].

In the following five subsections, irreducible representations of D_4, Q, C_8, $C_2 \times C_4$ and $C_2 \times C_2 \times C_2$ are found using Burnside method.

2.1 Irreducible Representations of Dihedral Group, D_4

The group D_4 is split up into five conjugacy classes as listed in Table 1, where the symbols C_1, C_2, ...,C_5 are labels used to distinguish the classes and the elements right below them are elements which make up the respective classes.

Table 1: Classes in D_4 and their elements

C_1	C_2	C_3	C_4	C_5
1	a, a^3	a^2	b, a^2b	ab, a^3b

The first step to obtain the irreducible representations is to use equation (1) to obtain the class multiplication coefficients. For instance, the class C_5 has two elements, namely ab and a^3b. The multiplication table of C_5 with C_5 is shown in Table 2.

Table 2: Multiplication table of C_5 with C_5

$\cdot$	ab	a^3b
ab	1	a^2
a^3b	a^2	1

Since 1 is the element of the class C_1 and a^2 is the element of the class C_3, the table shows that $C_5 \cdot C_5 = 2C_1 + 2C_3$.

Therefore, from (1),

$$\begin{aligned} C_5 \cdot C_5 &= c_{55,1}C_1 + c_{55,2}C_2 + c_{55,3}C_3 + c_{55,4}C_4 + c_{55,5}C_5, \text{ which gives} \\ 2C_1 + 2C_3 &= c_{55,1}C_1 + c_{55,2}C_2 + c_{55,3}C_3 + c_{55,4}C_4 + c_{55,5}C_5. \\ \text{This implies} \quad c_{55,1} &= 2 \quad \text{and} \quad c_{55,3} = 2. \end{aligned}$$

Evaluating equation (1) for all cases, the non-zero class multiplication coefficients are obtained as follows:

$c_{11,1} = 1$	$c_{22,1} = 2$	$c_{33,1} = 1$	$c_{44,1} = 2$	$c_{55,1} = 2$
$c_{12,2} = 1$	$c_{22,3} = 2$	$c_{34,4} = 1$	$c_{44,3} = 2$	$c_{55,3} = 2$
$c_{13,3} = 1$	$c_{23,2} = 1$	$c_{35,5} = 1$	$c_{45,2} = 2$	
$c_{14,4} = 1$	$c_{24,5} = 2$			
$c_{15,5} = 1$	$c_{25,4} = 2$			

Next, the characters of the irreducible representations in terms of d_k are found using equation (2). For example, in the case $i = j = 1$:

$$\begin{aligned} h_1h_1{\chi_1}^k{\chi_1}^k &= d_k \sum_{s=1}^{5} c_{11,s}h_s{\chi_s}^k \\ &= d_k(c_{11,1}h_1{\chi_1}^k + c_{11,2}h_2{\chi_2}^k + c_{11,3}h_3{\chi_3}^k + c_{11,4}h_4{\chi_4}^k + c_{11,5}h_5{\chi_5}^k) \\ &= d_k(c_{11,1}h_1{\chi_1}^k + (0)h_2{\chi_2}^k + (0)h_3{\chi_3}^k + (0)h_4{\chi_4}^k + (0)h_5{\chi_5}^k) \\ &= d_kc_{11,1}h_1{\chi_1}^k. \\ \text{Since} \quad c_{11,1} &= 1, h_1 = 1, \text{ thus, } {\chi_1}^k = d_k. \end{aligned}$$

Similarly, calculations in the case $i = j = 3$ will yield ${\chi_3}^k = \pm d_k$. Considering all calculations in the cases when $c_{ij,s} \neq 0$, $i, j, s = 1, \ldots, 5$, the following results are obtained:

For negative value of ${\chi_3}^k$, the values of ${\chi_2}^k$ and ${\chi_4}^k$ turn out to be 0. For positive values of ${\chi_3}^k$, we get the following results:

(i) if ${\chi_2}^k = d_k$, ${\chi_4}^k = d_k$, then ${\chi_5}^k = d_k$,

(ii) if ${\chi_2}^k = d_k$, ${\chi_4}^k = -d_k$, then ${\chi_5}^k = -d_k$,

(iii) if ${\chi_2}^k = -d_k$, ${\chi_4}^k = d_k$, then ${\chi_5}^k = -d_k$,

(iv) if ${\chi_2}^k = -d_k$, ${\chi_4}^k = -d_k$, then ${\chi_5}^k = d_k$.

All of these characters of the irreducible representations of D_4 are shown in Table 3, where entries in row i ($i = 1, \ldots, 5$) correspond to the ith irreducible representation.

Table 3: Characters of the irreducible representations of D_4 in terms of d_k

C_1	C_2	C_3	C_4	C_5
d_k	d_k	d_k	d_k	d_k
d_k	d_k	d_k	$-d_k$	$-d_k$
d_k	$-d_k$	d_k	d_k	$-d_k$
d_k	$-d_k$	d_k	$-d_k$	d_k
d_k	0	$-d_k$	0	0

Lastly, equation (3) is used to obtain the numerical values for d_k. For each $1 \leq k \leq 5$,

$$\begin{aligned}
\sum_{i=1}^{5} h_i({\chi_i}^k)^2 &= h_1{\chi_1}^k{\chi_1}^k + h_2{\chi_2}^k{\chi_2}^k + h_3{\chi_3}^k{\chi_3}^k + h_4{\chi_4}^k{\chi_4}^k + h_5{\chi_5}^k{\chi_5}^k \\
&= {\chi_1}^k{\chi_1}^k + 2{\chi_2}^k{\chi_2}^k + {\chi_3}^k{\chi_3}^k + 2{\chi_4}^k{\chi_4}^k + 2{\chi_5}^k{\chi_5}^k \\
&= 8.
\end{aligned}$$

For example, using the characters of the third irreducible representation, when $k = 3$,

$$\begin{aligned}
\sum_{i=1}^{5} h_i({\chi_i}^k)^2 &= d_3d_3 + 2(-d_3)(-d_3) + d_3d_3 + 2d_3d_3 + 2(-d_3)(-d_3) \\
&= 8{d_3}^2 \\
&= 8. \\
\text{Thus, } d_3 &= 1.
\end{aligned}$$

Therefore, $d_k = 1$ for the first four irreducible representations and $d_k = 2$ for the fifth irreducible representation. The characters of the five irreducible representations of D_4 are given in Table 4, where Γ_1, Γ_2, …, Γ_5 are labels for the different irreducible representations.

Thus for D_4, there are five irreducible representations.

Table 4: Irreducible representations of D_4

	C_1	C_2	C_3	C_4	C_5
Γ_1	1	1	1	1	1
Γ_2	1	1	1	-1	-1
Γ_3	1	-1	1	1	-1
Γ_4	1	-1	1	-1	1
Γ_5	2	0	-2	0	0

2.2 Irreducible Representations of Quaternion Group, Q

The group Q is split up into five conjugacy classes which are exactly the same as those for D_4, shown in Table 1. Therefore, the steps to obtain the irreducible representations of Q are similar to the one for D_4. The characters of the five irreducible representations of Q are exactly the same as those obtained for D_4, shown in Table 4.

2.3 Irreducible Representations of Cyclic Group of Order 8, C_8

The group C_8 is split up into eight conjugacy classes as listed in Table 5.

Table 5: Classes in C_8 and their elements

C_1	C_2	C_3	C_4	C_5	C_6	C_7	C_8
1	a	a^2	a^3	a^4	a^5	a^6	a^7

Evaluating equation (1) for all cases, the non-zero class multiplication coefficients are obtained as follows:

$c_{11,1} = 1$	$c_{22,3} = 1$	$c_{33,5} = 1$	$c_{44,7} = 1$	$c_{55,1} = 1$	$c_{66,3} = 1$	$c_{77,5} = 1$	$c_{88,7} = 1$
$c_{12,2} = 1$	$c_{23,4} = 1$	$c_{34,6} = 1$	$c_{45,8} = 1$	$c_{56,2} = 1$	$c_{67,4} = 1$	$c_{78,6} = 1$	
$c_{13,3} = 1$	$c_{24,5} = 1$	$c_{35,7} = 1$	$c_{46,1} = 1$	$c_{57,3} = 1$	$c_{68,5} = 1$		
$c_{14,4} = 1$	$c_{25,6} = 1$	$c_{36,8} = 1$	$c_{47,2} = 1$	$c_{58,4} = 1$			
$c_{15,5} = 1$	$c_{26,7} = 1$	$c_{37,1} = 1$	$c_{48,3} = 1$				
$c_{16,6} = 1$	$c_{27,8} = 1$	$c_{38,2} = 1$					
$c_{17,7} = 1$	$c_{28,1} = 1$						
$c_{18,8} = 1$							

Next, the characters of the irreducible representations in terms of d_k are found using equation (2). For example, in the case $i = j = 1$:

$$
\begin{aligned}
h_1h_1{\chi_1}^k{\chi_1}^k &= d_k\sum_{s=1}^{8} c_{11,s}h_s{\chi_s}^k \\
&= d_k(c_{11,1}h_1{\chi_1}^k + c_{11,2}h_2{\chi_2}^k + c_{11,3}h_3{\chi_3}^k + c_{11,4}h_4{\chi_4}^k \\
&\quad + c_{11,5}h_5{\chi_5}^k + c_{11,6}h_6{\chi_6}^k + c_{11,7}h_7{\chi_7}^k + c_{11,8}h_8{\chi_8}^k) \\
&= d_k((1)h_1{\chi_1}^k + (0)h_2{\chi_2}^k + (0)h_3{\chi_3}^k + (0)h_4{\chi_4}^k \\
&\quad + (0)h_5{\chi_5}^k + (0)h_6{\chi_6}^k + (0)h_7{\chi_7}^k + (0)h_8{\chi_8}^k) \\
&= d_kh_1{\chi_1}^k. \\
\text{Since } h_1 = 1, \ \text{ thus } {\chi_1}^k &= d_k. \\
h_5h_5{\chi_5}^k{\chi_5}^k &= d_k\sum_{s=1}^{8} c_{55,s}h_s{\chi_s}^k \\
&= d_k(c_{55,1}h_1{\chi_1}^k + c_{55,2}h_2{\chi_2}^k + c_{55,3}h_3{\chi_3}^k + c_{55,4}h_4{\chi_4}^k \\
&\quad + c_{55,5}h_5{\chi_5}^k + c_{55,6}h_6{\chi_6}^k + c_{55,7}h_7{\chi_7}^k + c_{55,8}h_8{\chi_8}^k) \\
&= d_k((1)h_1{\chi_1}^k + (0)h_2{\chi_2}^k + (0)h_3{\chi_3}^k + (0)h_4{\chi_4}^k \\
&\quad + (0)h_5{\chi_5}^k + (0)h_6{\chi_6}^k + (0)h_7{\chi_7}^k + (0)h_8{\chi_8}^k) \\
&= d_kh_1{\chi_1}^k. \\
\text{Since } \ h_1 = h_5 &= 1 \quad \text{and} \quad {\chi_1}^k = d_k, \quad \text{thus} \\
{\chi_5}^k{\chi_5}^k &= {d_k}^2, \\
{\chi_5}^k &= \pm d_k.
\end{aligned}
$$

Considering all cases when $c_{ij,s} \neq 0, i, j, s = 1, \ldots, 8$,

$$
\begin{aligned}
\text{if} \quad {\chi_5}^k &= d_k, \quad \text{then} \quad {\chi_3}^k = \pm d_k; \\
\text{if} \quad {\chi_5}^k &= -d_k, \quad \text{then} \quad {\chi_3}^k = \pm d_k i, \\
\text{if} \quad {\chi_3}^k &= d_k, \quad \text{then} \quad {\chi_6}^k = \pm d_k; \\
\text{if} \quad {\chi_3}^k &= -d_k, \quad \text{then} \quad {\chi_6}^k = \pm d_k i; \\
\text{if} \quad {\chi_3}^k &= d_k i, \quad \text{then} \quad {\chi_6}^k = \pm d_k \epsilon, \quad \text{where} \quad \epsilon = i^{\frac{1}{2}}; \\
\text{if} \quad {\chi_3}^k &= -d_k i, \quad \text{then} \quad {\chi_6}^k = \pm d_k \epsilon^*, \quad \text{where} \quad \epsilon^* = (-i)^{\frac{1}{2}},
\end{aligned}
$$

and the others can similarly be shown.

All of these characters of the irreducible representations of C_8 are shown in Table 6, where entries in row i ($i = 1, \ldots, 8$) correspond to the ith irreducible representation.

Lastly, equation (3) is used to obtain the numerical values for d_k. For each $1 \leq k \leq 8$,

$$
\begin{aligned}
\sum_{i=1}^{8} h_i({\chi_i}^k)^2 &= h_1{\chi_1}^k{\chi_1}^k + h_2{\chi_2}^k{\chi_2}^k + h_3{\chi_3}^k{\chi_3}^k + h_4{\chi_4}^k{\chi_4}^k \\
&\quad + h_5{\chi_5}^k{\chi_5}^k + h_6{\chi_6}^k{\chi_6}^k + h_7{\chi_7}^k{\chi_7}^k + h_8{\chi_8}^k{\chi_8}^k \\
&= {\chi_1}^k{\chi_1}^k + {\chi_2}^k{\chi_2}^k + {\chi_3}^k{\chi_3}^k + {\chi_4}^k{\chi_4}^k \\
&\quad + {\chi_5}^k{\chi_5}^k + {\chi_6}^k{\chi_6}^k + {\chi_7}^k{\chi_7}^k + {\chi_8}^k{\chi_8}^k \\
&= 8.
\end{aligned}
$$

Table 6: Characters of the irreducible representations of C_8 in terms of d_k

C_1	C_2	C_3	C_4	C_5	C_6	C_7	C_8
d_k	d_k	d_k	d_k	d_k	d_k	d_k	d_k
d_k	$-d_k$	d_k	$-d_k$	d_k	$-d_k$	d_k	$-d_k$
d_k	$d_k i$	$-d_k$	$-d_k i$	d_k	$d_k i$	$-d_k$	$-d_k i$
d_k	$-d_k i$	$-d_k$	$d_k i$	d_k	$-d_k i$	$-d_k$	$d_k i$
d_k	$d_k\epsilon$	$d_k i$	$-d_k\epsilon^*$	$-d_k$	$-d_k\epsilon$	$-d_k i$	$d_k\epsilon^*$
d_k	$-d_k\epsilon$	$d_k i$	$d_k\epsilon^*$	$-d_k$	$d_k\epsilon$	$-d_k i$	$-d_k\epsilon^*$
d_k	$d_k\epsilon^*$	$-d_k i$	$-d_k\epsilon$	$-d_k$	$-d_k\epsilon^*$	$d_k i$	$d_k\epsilon$
d_k	$-d_k\epsilon^*$	$-d_k i$	$d_k\epsilon$	$-d_k$	$d_k\epsilon^*$	$d_k i$	$-d_k\epsilon$

For the second to sixth irreducible representations, it is necessary to take the complex conjugate of ${\chi_i}^j$ since complex numbers are involved. For example, using the characters of the fifth irreducible representation, when $k = 5$,

$$\begin{aligned}
\sum_{i=1}^{8} h_i({\chi_i}^k)^2 &= (d_5)(\overline{d_5}) + (d_5\epsilon)(\overline{d_5\epsilon}) + (d_5 i)(\overline{d_5 i}) + (-d_5\epsilon^*)(\overline{-d_5\epsilon^*}) \\
&\quad + (-d_5)(\overline{-d_5}) + (-d_5\epsilon)(\overline{-d_5\epsilon}) + (-d_5 i)(\overline{-d_5 i}) + (d_5\epsilon^*)(\overline{d_5\epsilon^*}) \\
&= {d_5}^2(1 + (\epsilon)(\overline{\epsilon}) + (i)(\overline{i}) + (-\epsilon^*)(\overline{-\epsilon^*}) \\
&\quad + (-1)(\overline{-1}) + (-\epsilon)(\overline{-\epsilon}) + (-i)(\overline{-i}) + (\epsilon^*)(\overline{\epsilon^*})) \\
&= 8.
\end{aligned}$$

$$\begin{aligned}
\text{Since}\quad (\epsilon)(\overline{\epsilon}) &= 1,\ (\epsilon^*)(\overline{\epsilon^*}) = 1 \quad \text{and} \quad (i)(\overline{i}) = 1, \\
8{d_5}^2 &= 8, \\
d_5 &= 1.
\end{aligned}$$

For this group, $d_k = 1$, $1 \le k \le 8$, for all eight irreducible representations. Thus, the characters of the eight irreducible representations of C_8 are given in Table 7, where $\Gamma_1,\ \Gamma_2, \ldots, \Gamma_8$ have been relabelled for the different irreducible representations. Therefore, C_8 has eight irreducible representations.

2.4 Irreducible Representations of $C_2 \times C_4$

The group $C_2 \times C_4$ is split up into eight conjugacy classes as listed in Table 8.

Evaluating equation (1) for all cases, the non-zero class multiplication coefficients are obtained as follows:

$c_{11,1} = 1$	$c_{22,3} = 1$	$c_{33,1} = 1$	$c_{44,3} = 1$	$c_{55,1} = 1$	$c_{66,3} = 1$	$c_{77,1} = 1$	$c_{88,3} = 1$
$c_{12,2} = 1$	$c_{23,4} = 1$	$c_{34,2} = 1$	$c_{45,8} = 1$	$c_{56,2} = 1$	$c_{67,4} = 1$	$c_{78,2} = 1$	
$c_{13,3} = 1$	$c_{24,1} = 1$	$c_{35,7} = 1$	$c_{46,5} = 1$	$c_{57,3} = 1$	$c_{68,1} = 1$		
$c_{14,4} = 1$	$c_{25,6} = 1$	$c_{36,8} = 1$	$c_{47,6} = 1$	$c_{58,4} = 1$			
$c_{15,5} = 1$	$c_{26,7} = 1$	$c_{37,5} = 1$	$c_{48,7} = 1$				
$c_{16,6} = 1$	$c_{27,8} = 1$	$c_{38,6} = 1$					
$c_{17,7} = 1$	$c_{28,5} = 1$						
$c_{18,8} = 1$							

Next, the characters of the irreducible representations in terms of d_k are found using equation (2). All of these characters of the irreducible representations of $C_2 \times C_4$ are shown in Table 9, where entries in row i $(i = 1, \ldots, 8)$ correspond to the ith irreducible representation.

Lastly, equation (3) is used to obtain the numerical values for d_k. For this group, $d_k = 1$, $1 \leq k \leq 8$, for all eight irreducible representations. Thus, the characters of the eight irreducible representations of $C_2 \times C_4$ are given in Table 10.

Therefore, $C_2 \times C_4$ has eight irreducible representations.

2.5 Irreducible Representations of $C_2 \times C_2 \times C_2$

The group $C_2 \times C_2 \times C_2$ is split up into eight conjugacy classes as listed in Table 11.

Evaluating equation (1) for all cases, the non-zero class multiplication coefficients are obtained as follows:

$c_{11,1} = 1$	$c_{22,1} = 1$	$c_{33,1} = 1$	$c_{44,1} = 1$	$c_{55,1} = 1$	$c_{66,1} = 1$	$c_{77,1} = 1$	$c_{88,1} = 1$
$c_{12,2} = 1$	$c_{23,5} = 1$	$c_{34,7} = 1$	$c_{45,8} = 1$	$c_{56,7} = 1$	$c_{67,5} = 1$	$c_{78,2} = 1$	
$c_{13,3} = 1$	$c_{24,6} = 1$	$c_{35,2} = 1$	$c_{46,2} = 1$	$c_{57,6} = 1$	$c_{68,3} = 1$		
$c_{14,4} = 1$	$c_{25,3} = 1$	$c_{36,8} = 1$	$c_{47,3} = 1$	$c_{58,4} = 1$			
$c_{15,5} = 1$	$c_{26,4} = 1$	$c_{37,4} = 1$	$c_{48,5} = 1$				
$c_{16,6} = 1$	$c_{27,8} = 1$	$c_{38,6} = 1$					
$c_{17,7} = 1$	$c_{28,7} = 1$						
$c_{18,8} = 1$							

Next, the characters of the irreducible representations in terms of d_k are found using equation (2). All of these characters of the irreducible representations of $C_2 \times C_2 \times C_2$ are shown in Table 12, where entries in row i $(i = 1, \ldots, 8)$ correspond to the ith irreducible representation.

Lastly, equation (3) is used to obtain the numerical values for d_k. For this group, $d_k = 1$, $1 \leq k \leq 8$, for all eight irreducible representations. Thus, the characters of the eight irreducible representations of $C_2 \times C_2 \times C_2$ are given in Table 13.

Therefore, $C_2 \times C_2 \times C_2$ has eight irreducible representations.

In the next section, the second method, namely Great Orthogonality Theorem method is discussed to deduce irreducible representations of a group.

3 Great Orthogonality Theorem Method

The Great Orthogonality Theorem formula is stated as follows [3]:

$$\sum_R [\Gamma_i(R)_{mn}][\Gamma_j(R)_{m'n'}]^* = \frac{h}{\sqrt{l_i l_j}} \delta_{ij} \delta_{mm'} \delta_{nn'} \tag{4}$$

where h is the order of a group, l_i is the dimension of the ith representation, which is the order of each of the matrices which constitute it, R is the generic symbol given to the various operations in the group, $\Gamma_i(R)_{mn}$ is the element in the mth row and the nth column of the matrix corresponding to an operation R in the ith irreducible representation.

There are five important rules to find irreducible representations and their characters [3]:

Table 7: Irreducible representations of C_8

	C_1	C_2	C_3	C_4	C_5	C_6	C_7	C_8
Γ_1	1	1	1	1	1	1	1	1
Γ_2	1	-1	1	-1	1	-1	1	-1
Γ_3	1	i	-1	$-i$	1	i	-1	$-i$
Γ_4	1	$-i$	-1	i	1	$-i$	-1	i
Γ_5	1	ϵ	i	$-\epsilon^*$	-1	$-\epsilon$	$-i$	ϵ^*
Γ_6	1	$-\epsilon$	i	ϵ^*	-1	ϵ	$-i$	$-\epsilon^*$
Γ_7	1	ϵ^*	$-i$	$-\epsilon$	-1	$-\epsilon^*$	i	ϵ
Γ_8	1	$-\epsilon^*$	$-i$	ϵ	-1	ϵ^*	i	$-\epsilon$

Table 8: Classes in $C_2 \times C_4$ and their elements

C_1	C_2	C_3	C_4	C_5	C_6	C_7	C_8
1	b	b^2	b^3	a	ba	b^2a	b^3a

Table 9: Characters of the irreducible representations of $C_2 \times C_4$ in terms of d_k

C_1	C_2	C_3	C_4	C_5	C_6	C_7	C_8
d_k	d_k	d_k	d_k	d_k	d_k	d_k	d_k
d_k	$-d_k$	d_k	$-d_k$	d_k	$-d_k$	d_k	$-d_k$
d_k	d_ki	$-d_k$	$-d_ki$	d_k	d_ki	$-d_k$	$-d_ki$
d_k	$-d_ki$	$-d_k$	d_ki	d_k	$-d_ki$	$-d_k$	d_ki
d_k	d_k	d_k	d_k	$-d_k$	$-d_k$	$-d_k$	$-d_k$
d_k	$-d_k$	d_k	$-d_k$	$-d_k$	d_k	$-d_k$	d_k
d_k	d_ki	$-d_k$	$-d_ki$	$-d_k$	$-d_ki$	d_k	d_ki
d_k	$-d_ki$	$-d_k$	d_ki	$-d_k$	d_ki	d_k	$-d_ki$

Table 10: Irreducible representations of $C_2 \times C_4$

	C_1	C_2	C_3	C_4	C_5	C_6	C_7	C_8
Γ_1	1	1	1	1	1	1	1	1
Γ_2	1	-1	1	-1	1	-1	1	-1
Γ_3	1	i	-1	$-i$	1	i	-1	$-i$
Γ_4	1	$-i$	-1	i	1	$-i$	-1	i
Γ_5	1	1	1	1	-1	-1	-1	-1
Γ_6	1	-1	1	-1	-1	1	-1	1
Γ_7	1	i	-1	$-i$	-1	$-i$	1	i
Γ_8	1	$-i$	-1	i	-1	i	1	$-i$

Table 11: Classes in $C_2 \times C_2 \times C_2$ and their elements

C_1	C_2	C_3	C_4	C_5	C_6	C_7	C_8
1	a	b	c	ab	ac	bc	abc

Table 12: Characters of the irreducible representations of $C_2 \times C_2 \times C_2$ in terms of d_k

C_1	C_2	C_3	C_4	C_5	C_6	C_7	C_8
d_k	d_k	d_k	d_k	d_k	d_k	d_k	d_k
d_k	d_k	d_k	$-d_k$	d_k	$-d_k$	$-d_k$	$-d_k$
d_k	d_k	$-d_k$	$-d_k$	$-d_k$	$-d_k$	d_k	d_k
d_k	d_k	$-d_k$	d_k	$-d_k$	d_k	$-d_k$	$-d_k$
d_k	$-d_k$	d_k	d_k	$-d_k$	$-d_k$	d_k	$-d_k$
d_k	$-d_k$	d_k	$-d_k$	$-d_k$	d_k	$-d_k$	d_k
d_k	$-d_k$	$-d_k$	$-d_k$	d_k	d_k	d_k	$-d_k$
d_k	$-d_k$	$-d_k$	d_k	d_k	$-d_k$	$-d_k$	d_k

Table 13: Irreducible representations of $C_2 \times C_2 \times C_2$

	C_1	C_2	C_3	C_4	C_5	C_6	C_7	C_8
Γ_1	1	1	1	1	1	1	1	1
Γ_2	1	1	1	-1	1	-1	-1	-1
Γ_3	1	1	-1	-1	-1	-1	1	1
Γ_4	1	1	-1	1	-1	1	-1	-1
Γ_5	1	-1	1	1	-1	-1	1	-1
Γ_6	1	-1	1	-1	-1	1	-1	1
Γ_7	1	-1	-1	-1	1	1	1	-1
Γ_8	1	-1	-1	1	1	-1	-1	1

Rule 1: The sum of the squares of the dimensions of the irreducible representations of a group is equal to the order of the group, that is,

$$\sum {l_i}^2 = {l_1}^2 + {l_2}^2 + {l_3}^2 + \ldots = h \tag{5}$$

where l_i is the dimension of the ith representation and h is the order of a group.

Rule 2: The sum of the squares of the characters in any irreducible representation equals the order of the group, that is,

$$\sum_R [\chi_i(R)]^2 = h \tag{6}$$

where R is the various operations in the group, $\chi_i(R)$ is the character of the representation of R in the ith irreducible representation and h is the order of the group.

Rule 3: The vectors whose components are the characters of two different irreducible representations are orthogonal, that is,

$$\sum_R \chi_i(R)\chi_j(R) = 0 \quad \text{when} \quad i \neq j \tag{7}$$

where $\chi_i(R)$ is the character of the representation of R in the ith irreducible representation.

Rule 4: In a given representation (reducible or irreducible), the characters of all matrices belonging to operations in the same class are identical.

Rule 5: The number of irreducible representations of a group is equal to the number of classes in the group.

There is a specific method to find the irreducible representations for cyclic groups using this method. A cyclic group is Abelian and each of its h elements is in a separate class. It also has h 1-dimensional irreducible representations. In order to obtain the irreducible representations for a cyclic group, the exponential below is used as the pth irreducible representation, $\Gamma_p(C_n)$:

$$\epsilon^p = \exp\left(\frac{2\pi i p}{n}\right) = \cos\frac{2\pi p}{n} + i\sin\frac{2\pi p}{n} \tag{8}$$

where C_n is the cyclic group of order n and $p = 1, \ldots, n$. A table is obtained where the elements inside are obtained by group multiplication. Then the powers of ϵ's are reduced to modulo 8. Finally, the elements in the table are replaced with their values using equation (8). Thus the irreducible representations of the group are obtained.

Moreover, using this method, for groups which is made up of direct product of two (or more) groups, say $C_m \times C_n$, the representations of C_m is determined by the mth roots of unity and the representations of C_n is determined by the nth roots of unity. In other words, if χ and δ are the mth and nth roots of unity determining certain irreducible representations of the groups C_m and C_n, then the pair $\{\chi, \delta\}$ determine an irreducible representation T of $C_m \times C_n$ through the formula below [4]:

$$T[(a^i, b^j)] = \chi^i \delta^j \tag{9}$$

In the following five subsections, irreducible representations of D_4, Q, C_8, $C_2 \times C_4$ and $C_2 \times C_2 \times C_2$ are found using Great Orthogonality Theorem method.

3.1 Irreducible Representations of Dihedral Group, D_4

According to rule 5, since the group D_4 consists of five classes, there are five irreducible representations for this group. By rule 1, we find a set of five positive integers, l_1, l_2, l_3, l_4 and l_5 which satisfy the equation ${l_1}^2 + {l_2}^2 + {l_3}^2 + {l_4}^2 + {l_5}^2 = 8$. The only values of l_i (i=1,...,5) which satisfy this requirement are 1, 1, 1, 1 and 2. Thus, the group D_4 has four 1-dimensional irreducible representations and one 2-dimensional irreducible representation. By rule 2, in any group, there will be a 1-dimensional irreducible representation whose characters are all equal to 1, since

$$\sum_R (\chi_1(R))^2 = (1)1^2 + (2)1^2 + (1)1^2 + (2)1^2 + (2)1^2 = 8.$$

The other representations will have to be such that $\sum_R (\chi_i(R))^2 = 8$, which can be true if and only if each $\chi_i(R) = \pm 1$. By rule 3, each of the other three representations has to be orthogonal to the first irreducible representation, Γ_1. Thus, there will have to be two $+1$'s and two -1's. The fifth representation will be of dimension 2, hence $\chi_5(C_1) = 2$. In order to find out the values of $\chi_5(C_2)$, $\chi_5(C_3)$, $\chi_5(C_4)$ and $\chi_5(C_5)$, the orthogonality relationships as stated by equation (7) in rule 3 is used. Solving the four simultaneous equations below:

$$\begin{aligned}
\sum_R \chi_1(R)\chi_5(R) &= (1)(2) + (1)\chi_5(C_2) + (1)\chi_5(C_3) + (1)\chi_5(C_4) + (1)\chi_5(C_5) = 0, \\
\sum_R \chi_2(R)\chi_5(R) &= (1)(2) + (1)\chi_5(C_2) + (1)\chi_5(C_3) + (-1)\chi_5(C_4) + (-1)\chi_5(C_5) = 0, \\
\sum_R \chi_3(R)\chi_5(R) &= (1)(2) + (-1)\chi_5(C_2) + (1)\chi_5(C_3) + (1)\chi_5(C_4) + (-1)\chi_5(C_5) = 0, \\
\sum_R \chi_4(R)\chi_5(R) &= (1)(2) + (-1)\chi_5(C_2) + (1)\chi_5(C_3) + (-1)\chi_5(C_4) + (1)\chi_5(C_5) = 0,
\end{aligned}$$

gives $\chi_5(C_2) = \chi_5(C_4) = \chi_5(C_5) = 0$ and $\chi_5(C_3) = -2$.

The complete set of irreducible representations of D_4 is found to be the same as those in Table 4.

3.2 Irreducible Representations of Quaternion Group, Q

The steps to obtain the irreducible representations of Q are exactly the same as those for D_4. Therefore, the complete set of irreducible representations of Q is also shown in Table 4.

3.3 Irreducible Representations of Cyclic Group of Order 8, C_8

According to rule 5, since the group C_8 consists of eight classes, there are eight irreducible representations for this group. By rule 1, using equation (5), ${l_1}^2 + {l_2}^2 + {l_3}^2 + {l_4}^2 + {l_5}^2 + {l_6}^2 + {l_7}^2 + {l_8}^2 = 8$. Therefore, possible values for l_i $(i = 1, ..., 8)$ are all 1s. In other words, the group C_8 has a set of eight 1-dimensional irreducible representations namely, Γ_1, Γ_2, Γ_3, Γ_4, Γ_5, Γ_6, Γ_7 and Γ_8 which satisfy

$$\sum_{m=1}^{8} [\Gamma_p({C_n}^m)][\Gamma_q({C_n}^m)]^* = h\delta_{pq}. \tag{10}$$

Since this is a cyclic group, the exponential below is used:

$$\begin{aligned}\Gamma_p(C_8) &= \epsilon^p \\ &= \exp(\frac{2\pi ip}{8}) \\ &= \cos(\frac{2\pi p}{8}) + i\sin(\frac{2\pi p}{8})\end{aligned}$$

Table 14 shows the set where the elements inside the table are obtained by group multiplication:

Table 14: Table whose elements are obtained by group multiplication

	C_1	C_2	C_3	C_4	C_5	C_6	C_7	C_8
Γ_1	ϵ^8	ϵ	ϵ^2	ϵ^3	ϵ^4	ϵ^5	ϵ^6	ϵ^7
Γ_2	ϵ^{16}	ϵ^2	ϵ^4	ϵ^6	ϵ^8	ϵ^{10}	ϵ^{12}	ϵ^{14}
Γ_3	ϵ^{24}	ϵ^3	ϵ^6	ϵ^9	ϵ^{12}	ϵ^{15}	ϵ^{18}	ϵ^{21}
Γ_4	ϵ^{32}	ϵ^4	ϵ^8	ϵ^{12}	ϵ^{16}	ϵ^{20}	ϵ^{24}	ϵ^{28}
Γ_5	ϵ^{40}	ϵ^5	ϵ^{10}	ϵ^{15}	ϵ^{20}	ϵ^{25}	ϵ^{30}	ϵ^{35}
Γ_6	ϵ^{48}	ϵ^6	ϵ^{12}	ϵ^{18}	ϵ^{24}	ϵ^{30}	ϵ^{36}	ϵ^{42}
Γ_7	ϵ^{56}	ϵ^7	ϵ^{14}	ϵ^{21}	ϵ^{28}	ϵ^{35}	ϵ^{42}	ϵ^{49}
Γ_8	ϵ^{64}	ϵ^8	ϵ^{16}	ϵ^{24}	ϵ^{32}	ϵ^{40}	ϵ^{48}	ϵ^{56}

In order to show that these representations satisfy equation (10), consider any two representations, say Γ_p and Γ_q, where $q - p = r$. The left-hand side of equation (10) is

$$\begin{aligned}(\epsilon^p)^*\epsilon^{p+r} + (\epsilon^{2p})^*\epsilon^{2(p+r)} + (\epsilon^{3p})^*\epsilon^{3(p+r)} + (\epsilon^{4p})^*\epsilon^{4(p+r)} \\ +(\epsilon^{5p})^*\epsilon^{5(p+r)} + (\epsilon^{6p})^*\epsilon^{6(p+r)} + (\epsilon^{7p})^*\epsilon^{7(p+r)} + (\epsilon^{8p})^*\epsilon^{8(p+r)}\end{aligned}$$

which can be simplified as

$$\epsilon^r + \epsilon^{2r} + \epsilon^{3r} + \epsilon^{4r} + \epsilon^{5r} + \epsilon^{6r} + \epsilon^{7r} + \epsilon^{8r} = \sum_{s=1}^{8} \exp(\frac{2\pi is}{8}). \quad (11)$$

The representation are thus normalized, since if $\Gamma_p = \Gamma_q$, then $r = 0$ and equation (11) is eight times e^0, that is 8. If Γ_p and Γ_q are different, r is some number from 1 to 7 since ϵ^8 equal to 1.

Therefore, the sum of equation (11) reduces to 0, that is,

$$\sum_{s=1}^{8} \exp(\frac{2\pi is}{8}) = 0$$

using the trigonometric identities

$$\sum_{s=1}^{l} \cos\frac{2\pi s}{l} = 0 \quad \text{and} \quad \sum_{s=1}^{l} \sin\frac{2\pi s}{l} = 0.$$

Table 15: Reducing the powers of ϵ's to modulo 8 to Table 14

	C_1	C_2	C_3	C_4	C_5	C_6	C_7	C_8
Γ_1	1	ϵ	ϵ^2	ϵ^3	ϵ^4	ϵ^5	ϵ^6	ϵ^7
Γ_2	1	ϵ^2	ϵ^4	ϵ^6	1	ϵ^2	ϵ^4	ϵ^6
Γ_3	1	ϵ^3	ϵ^6	ϵ	ϵ^4	ϵ^7	ϵ^2	ϵ^5
Γ_4	1	ϵ^4	1	ϵ^4	1	ϵ^4	1	ϵ^4
Γ_5	1	ϵ^5	ϵ^2	ϵ^7	ϵ^4	ϵ	ϵ^6	ϵ^3
Γ_6	1	ϵ^6	ϵ^4	ϵ^2	1	ϵ^6	ϵ^4	ϵ^2
Γ_7	1	ϵ^7	ϵ^6	ϵ^5	ϵ^4	ϵ^3	ϵ^2	ϵ
Γ_8	1	1	1	1	1	1	1	1

Table 15 is set by reducing the powers of ϵ's to modulo 8.

Using equation (8) where ϵ^2 is replaced by i, ϵ^3 by $-\epsilon^*$, ϵ^4 by -1, ϵ^5 by $-\epsilon$, ϵ^6 by $-i$, ϵ^7 by ϵ^*, ϵ^8 by 1 and rearranging the rows, the characters of the eight irreducible representations of C_8 are the same as in Table 7.

3.4 Irreducible Representations of $C_2 \times C_4$

According to rule 5, since the group $C_2 \times C_4$ consists of eight classes, there are eight irreducible representations for this group. By rule 1, using equation (5), ${l_1}^2 + {l_2}^2 + {l_3}^2 + {l_4}^2 + {l_5}^2 + {l_6}^2 + {l_7}^2 + {l_8}^2 = 8$. Therefore, possible values for l_i $(i = 1, ..., 8)$ are all 1s. In other words, the group C_8 has a set of eight 1-dimensional irreducible representations namely, Γ_1, Γ_2, Γ_3, Γ_4, Γ_5, Γ_6, Γ_7 and Γ_8. Since this is a direct product group, the following approach is used.

The representations of C_2 are determined by square roots of unity: 1 and -1, and those of C_4 are determined by the fourth roots of unity: 1, i, -1 and $-i$. If χ and δ are second and fourth roots of unity determining certain irreducible representations of C_2 and C_4, then the pair $\{\chi, \delta\}$ determine an irreducible representation T of $C_2 \times C_4$ through the formula

$$T[(a^i, b^j)] \quad = \quad \chi^i \delta^j.$$

As an example, for the pair $\{-1, -i\}$,

$$\begin{aligned}
T[(a^0, b^0)] = (-1)^0(-i)^0 &= 1, \\
T[(a^0, b^1)] = (-1)^0(-i)^1 &= -i, \\
T[(a^0, b^2)] = (-1)^0(-i)^2 &= -1, \\
T[(a^0, b^3)] = (-1)^0(-i)^3 &= i, \\
T[(a^1, b^0)] = (-1)^1(-i)^0 &= -1, \\
T[(a^1, b^1)] = (-1)^1(-i)^1 &= i, \\
T[(a^1, b^2)] = (-1)^1(-i)^2 &= 1, \\
T[(a^1, b^3)] = (-1)^1(-i)^3 &= -i.
\end{aligned}$$

Continuing in this manner and rearranging the rows of irreducible representations, the characters of the eight irreducible representations of $C_2 \times C_4$ are found as in Table 10.

3.5 Irreducible Representations of $C_2 \times C_2 \times C_2$

As before, the group C_8 has a set of eight 1-dimensional irreducible representations namely, Γ_1, Γ_2, Γ_3, Γ_4, Γ_5, Γ_6, Γ_7 and Γ_8.

Since this group is a direct product of three copies of C_2, the same approach is used as for direct product of the groups C_2 with C_4.

The representations of C_2 are determined by square roots of unity: 1 and -1. If χ, δ and ϵ are all second roots of unity determining certain irreducible representations of C_2, then the pair $\{\chi, \delta, \epsilon\}$ determine an irreducible representation T of $C_2 \times C_2 \times C_2$ through the formula

$$T[(a^i, b^j, c^k)] \quad = \quad \chi^i \delta^j \epsilon^k.$$

As an example, for the pair $\{-1, -1, 1\}$,

$$\begin{aligned}
T[(a^0, b^0, c^0)] = (-1)^0(-1)^0 1^0 &= 1, \\
T[(a^1, b^0, c^0)] = (-1)^1(-1)^0 1^0 &= -1, \\
T[(a^0, b^1, c^0)] = (-1)^0(-1)^1 1^0 &= -1, \\
T[(a^0, b^0, c^1)] = (-1)^0(-1)^0 1^1 &= 1, \\
T[(a^1, b^1, c^0)] = (-1)^1(-1)^1 1^0 &= 1, \\
T[(a^1, b^0, c^1)] = (-1)^1(-1)^0 1^1 &= -1, \\
T[(a^0, b^1, c^1)] = (-1)^0(-1)^1 1^1 &= -1, \\
T[(a^1, b^1, c^1)] = (-1)^1(-1)^1 1^1 &= 1.
\end{aligned}$$

Continuing in this manner and rearranging the rows of irreducible representations, the characters of the eight irreducible representations of $C_2 \times C_2 \times C_2$ are found as in Table 13.

In the next section, Burnside method and Great Orthogonality Theorem method are compared.

4 Comparison of the Two Methods

Both Burnside method and Great Orthogonality Theorem method can be used to obtain the irreducible representations of all groups of order 8. Using Burnside method, three formulas are involved to find the irreducible representations. The first and second formulas are quite lengthy since there are $n!$ calculations for each formula for a group with n classes. Besides, every equation has to be satisfied in the second formula to find the characters of the irreducible representations in terms of d_k. As for the third formula, since it involves Kronecker Delta, only the cases when $j = k$ have to be checked. So there are only n calculations to be done for a group with n classes. It is necessary to take the complex conjugate of ${\chi_i}^j$, the character of the elements in class C_i in the irreducible representation labelled by j, whenever imaginary or complex numbers are involved. Burnside method can be applied to any groups without considering the structure of the group as in Great Orthogonality Theorem method.

For Great Orthogonality Theorem method, Great Orthogonality Theorem formula and five important rules concerning irreducible representations and their characters are used. However, for cyclic groups and direct product groups, there are certain steps to be followed to obtain the irreducible representations in addition to the Great Orthogonality Theorem formula and the five important rules. In general, this method is not as lengthy as Burnside method. Therefore, in order to deduce the irreducible representations for groups using Great Orthogonality Theorem method, the type of groups need to be identified first.

5 Applications

Identifying the irreducible representations associated with a given atom is of great value as convenient ways of labeling orbitals for reference, determining which sets of atomic orbitals can combine with each other to form molecular orbitals and for determining the number and nature of vibrational motions for a given molecule by removing the irreducible representations that correspond to the translation and rotation of the molecule. The properties of group presentations and their characters are also important in dealing with problems in valence theory and molecular dynamics.

6 Conclusions

Two of the methods to obtain the irreducible representations of a group are Burnside method and Great Orthogonality Theorem method. The two methods are used to obtain the irreducible representations of all groups of order 8 and comparison of the two methods are made. Although quite lengthy, Burnside method can be applied to any type of groups without having to consider the structure of the group. Great Orthogonality Theorem method is not as lengthy as Burnside method but there is specific method for cyclic groups and direct product groups in addition to the Great Orthogonality Theorem formula and the five important rules.

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